

Quantum shock waves in the Heisenberg XY model

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Abstract

We show the existence of quantum states of the Heisenberg XY chain which closely follow the motion of the corresponding semi-classical ones, and whose evolution resemble the propagation of a shock wave in a fluid. These states are exact solutions of the Schrödinger equation of the XY model and their classical counterpart are simply domain walls or soliton-like solutions.

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I. INTRODUCTION

The relationship between classical and quantum dynamics, although largely investigated since the beginning of quantum mechanics, is still a non exhausted problem of ever continuing interest. This has lead, for example, to the introduction of new concepts such as coherent states and their generalizations, which has been found to be successful in describing the quasiclassical behaviors of a wide class of physical problems. The possibility to construct quantum states which closely resemble the evolution of classical ones is appealing also in connection with the new developing area of quantum computing [1]. In this context the basic component of a quantum computer is a q-bit i.e. a special quantum state which has to be manipulated by the logical quantum gates (unitary operators) and which has to be preserved ‘intact’ for an extended period of time. In any practical task, however, the interaction of the system with the environment (heat reservoir) is unavoidable and decoherence usually develops. On the other hand, one may expect that, due to their intrinsic collective character, quantum states close to macroscopic (classical) ones are more robust against decoherence and therefore more suitable to store information in a quantum computer. The problem of finding such states, however, is far from being trivial even for isolated systems. Indeed, the complexity of a quantum system related to the huge dimensionality of the Hilbert space, represents a major obstacle in solving the time-dependent Schrödinger equation (one usually resorts to approximations which are not always well controlled).

The aim of the present paper is to show that for the XY Heisenberg spin chain [2] it is possible to find quantum states which closely follow the motion of the corresponding classical ones and whose evolution resemble the propagation of a shock wave in a fluid. The classical counterpart of these states are moving domain walls or soliton-like solutions. Stable shock-wave solutions of different shapes were also encountered in the semiclassical dynamics of the Heisenberg chain [3] as well as in other similar models [4]. Here we show, on the example of the solvable XY model, that a spin system may indeed have exact quantum states which recall classical moving shock-wave solutions. In particular, a detailed comparison between

the quantum and the classical evolution for several initial conditions is presented. The regions where the exact quantum states are well approximated by the classical ones are also investigated. In these regions the classical approach can be used to track the dynamics of those quantum observables which are technically inaccessible by a quantum-mechanical analysis. The paper is organized as follows. First we derive semiclassical and quantum equations of motion, and in particular solve them in the quantum case. This enables us to compare exact quantum and semiclassical time evolutions for a chosen set of initial conditions leading to shock-wave formation. The properties of the latter are then discussed, and in the conclusion the main results of the paper are summarized.

II. SEMICLASSICAL ANALYSIS OF THE XY MODEL

The quantum Heisenberg XY model ¹ is introduced as

$$\mathcal{H} = J \sum_n (s_n^x s_{n+1}^x + s_n^y s_{n+1}^y) \quad (1)$$

where $s^i = \frac{1}{2}\sigma^i$, $i = 1, 2, 3$ are spin $1/2$ operators, σ^i are Pauli matrices, and J is the exchange constant related to the interaction between spins. As well known, the two-dimensional character of the interaction and its restriction to neighbouring spins leads to the exact solvability of this model [5]. In the following we shall derive semiclassical equations of motion of the XY model, by averaging the Heisenberg equation of motion $i\hbar \frac{\partial \hat{f}}{\partial t} = [\hat{f}, \mathcal{H}]$ for a generic observable \hat{f} over (uncorrelated) coherent states. For s_n^z (site magnetization) and $s^\pm = s^x \pm is^y$ (rising and lowering operators), we have:

$$i\hbar \frac{\partial s_n^z}{\partial t} = \frac{J}{2} (s_n^+ s_{n+1}^- - s_n^- s_{n+1}^+ - s_{n-1}^+ s_n^- + s_{n-1}^- s_n^+), \quad (2)$$

$$-i\hbar \frac{\partial s_n^\pm}{\partial t} = \pm J s_n^z (s_{n+1}^\pm + s_{n-1}^\pm), \quad (3)$$

¹An arbitrary constant magnetic field $B \sum_n s_n^z$ can be included; here we consider $B = 0$ for simplicity.

(in the following to simplify notation we fix $\hbar = 1$ and $J = 1$). Introducing spin $\frac{1}{2}$ coherent states as

$$|\Lambda(t)\rangle = \prod_n \otimes |\mu_n(t)\rangle, \quad |\mu_n(t)\rangle = \frac{e^{\mu_n(t)s_n^-}}{\sqrt{1 + |\mu_n(t)|^2}} |\uparrow\rangle, \quad (4)$$

with $|\uparrow\rangle_n$ denoting the spin up state at site n , we compute

$$\langle s_n^+ \rangle = \frac{\mu_n}{1 + |\mu_n|^2}, \quad \langle s_n^- \rangle = \frac{\mu_n^*}{1 + |\mu_n|^2}, \quad \langle s_n^z \rangle = \frac{1}{2} \left(\frac{1 - |\mu_n|^2}{1 + |\mu_n|^2} \right), \quad (5)$$

where $\langle s \rangle$ denotes the average over the state $|\Lambda\rangle$. It is worth noting that these equations define an inverse stereographic mapping from the variables μ_n, μ_n^* , to the vectors \vec{S}_n (classical spins) on the unit sphere

$$S_n^x = \frac{\langle s_n^+ \rangle + \langle s_n^- \rangle}{2}, \quad S_n^y = \frac{\langle s_n^+ \rangle - \langle s_n^- \rangle}{2}, \quad S_n^z = \langle s_n^z \rangle \quad (6)$$

By averaging Eqs. (2), (3) with respect to $|\Lambda\rangle$ and by eliminating redundancy (note that the quantities in Eq. (5) are not all independent), we finally obtain the equation of motion for $\mu_n(t)$ as

$$i \frac{\partial \mu_n}{\partial t} = \frac{1}{2} \left(\frac{\mu_{n+1} - \mu_n^2 \mu_{n+1}^*}{1 + |\mu_{n+1}|^2} + \frac{\mu_{n-1} - \mu_n^2 \mu_{n-1}^*}{1 + |\mu_{n-1}|^2} \right). \quad (7)$$

Note that this equation (and its complex conjugated) can be put in hamiltonian form

$$\dot{\mu}_n = \{\mu_n, H\} \quad (8)$$

with respect to the Poisson bracket

$$\{f, g\} = -i \sum_n (1 + |\mu_n|^2)^2 \left(\frac{\partial f}{\partial \mu_n} \frac{\partial g}{\partial \mu_n^*} - \frac{\partial f}{\partial \mu_n^*} \frac{\partial g}{\partial \mu_n} \right), \quad (9)$$

and the hamiltonian

$$H_c(\mu, \mu^*) = \frac{1}{2} \sum_n \frac{\mu_{n+1}^* \mu_n + \mu_n^* \mu_{n+1}}{(1 + |\mu_n|^2)(1 + |\mu_{n+1}|^2)}. \quad (10)$$

These results were also derived in Ref. [3] using the stationary phase approximation and the path integral formulation of quantum mechanics. It is remarkable that the classical

hamiltonian in Eq. (10), once expressed in terms of the vectors \vec{S}_n through Eqs. (5,6), takes exactly the same form as in Eq. (1) with quantum operators replaced by classical spins. This is precisely what one would expect from the classical limit in coherent state representation. On the other hand, since coherent states do not preserve the hidden symmetry algebra of the quantum XY chain (they are not eigenstates of the monodromy operator) [6], the integrability structure of the system is lost in the semiclassical limit.

III. EXACT QUANTUM ANALYSIS OF THE XY MODEL

In this section we shall derive exact analytical expressions for the time evolution of the expectation values $\langle \hat{f}(t) \rangle = \langle \psi_0 | e^{i\mathcal{H}t} \hat{f}(0) e^{-i\mathcal{H}t} | \psi_0 \rangle$ of observables $\hat{f}(t)$ of the XY model. To this end we take as initial state $|\psi_0\rangle$ the totally uncorrelated quantum state

$$|\psi_0\rangle = \prod_{n=-\infty}^{\infty} \otimes \begin{pmatrix} e^{i\Phi_n/2} \cos(\alpha_n) \\ e^{-i\Phi_n/2} \sin(\alpha_n) \end{pmatrix}. \quad (11)$$

By the Jordan-Wigner [7] transformation from spin to Fermi operators

$$s_n^+ = \prod_{m < n} (1 - 2C_m^+ C_m) C_n, \quad s_n^- = (s_n^+)^*, \quad s_n^z = \frac{1}{2} - C_n^+ C_n, \quad (12)$$

the XY Hamiltonian (1) reduces to

$$\mathcal{H} = \frac{1}{2} \sum_n (C_{n+1}^+ C_n + C_n^+ C_{n+1}). \quad (13)$$

This Hamiltonian is readily diagonalized as

$$\mathcal{H} = \sum_k \cos(k) c_k^+ c_k, \quad (14)$$

by the Fourier transform $C_n = \frac{1}{\sqrt{N}} \sum_k e^{-ikn} c_k$. The Heisenberg equations of motion

$$i \frac{\partial c_k}{\partial t} = \cos(k) c_k, \quad (15)$$

are then solved as $c_k(t) = e^{-it\cos(k)} c_k(0)$. Returning to the operators C_n , we get

$$C_n(t) = \frac{1}{\sqrt{N}} \sum_k e^{-ikn - i\cos(k)t} c_k(0) = \sum_m i^{m-n} J_{m-n}(-t) C_m(0), \quad (16)$$

with $J_n(t)$ denoting the Bessel function of order n . From Eq. (12) and from its inverse

$$C_n = \left(\prod_{m < n} s_m^z \right) s_n^+, \quad C_n^+ = s_n^- \left(\prod_{m < n} s_m^z \right), \quad (17)$$

one can finally derive exact expressions for the time evolution of the observables of the original spin chain. Thus, for example, the time evolution of the averaged spin- z projection is obtained as

$$\begin{aligned} S_p^z(t) &\equiv 2\langle s_p^z \rangle = \langle \psi_0 | 1 - 2C_p^+(t)C_p(t) | \psi_0 \rangle = \\ &1 - 2 \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} i^{n-m} J_{n-p}(-t) J_{m-p}(-t) \langle \psi_0 | s_m^- \left(\prod_{l=-\infty}^{m-1} s_l^z \right) \left(\prod_{l'=-\infty}^{n-1} s_{l'}^z \right) s_n^+ | \psi_0 \rangle = \\ &S_p^z(0) - \sum_{n < m} J_n(t) J_m(t) \sin(2\alpha_{p+n}) \sin(2\alpha_{q+n}) \cos \left(\frac{\pi}{2} (m-n) + \Phi_{m+p} - \Phi_{n+p} \right) \prod_{j=n+p+1}^{m+p-1} S_j^z(0) \end{aligned} \quad (18)$$

(in a similar manner one proceeds for the other observables). In the next section we shall compare this expression for the average site magnetization, with direct numerical integrations of Eq. (7).

IV. COMPARISON BETWEEN CLASSICAL AND QUANTUM EVOLUTIONS

To compare the classical and quantum time evolution from an identical initial state, we shall first derive the classical initial conditions which correspond to the quantum state Eq. (11). To this end we remark that the expectation values of the operators s_n^\pm, s_n^z , with respect to $|\psi_0\rangle$ are easily calculated as

$$\langle s_n^\pm \rangle = \frac{e^{\mp i\Phi_n}}{2} \sin 2\alpha_n, \quad \langle s_n^z \rangle = \frac{1}{2} \cos 2\alpha_n. \quad (19)$$

The initial conditions in the classical system are fixed by requiring that the above expressions for $\langle s_n^\pm \rangle, \langle s_n^z \rangle$, coincide with the corresponding classical ones in Eq. (5), this leading to

$$\mu_n(0) = tg(\alpha_n) e^{-i\Phi_n} \quad (20)$$

as initial conditions for Eq.7. Since the classical states stay uncorrelated for all times while quantum ones develop correlations in the course of time, one expects the corresponding

classical and quantum time evolution to be different for generic initial conditions. For special choices of the initial conditions however, these dynamics may qualitatively agree for times long enough to observe phenomena of the classical system, such as shock waves formation, also in the quantum one. Shock waves were observed in a semiclassical description of the Heisenberg chain using as initial conditions non constant (bell shaped) profiles for $\langle s_n^z \rangle$ with a constant phase $\Phi_n = \text{const}$ along the chain [3]. Here it is convenient to take as initial conditions constant values for the site magnetizations but not for the phase i.e. we use

$$S_n^z(0) = \cos(2\alpha), \quad \Phi_n = \Phi(n), \quad -\frac{N}{2} \leq n \leq \frac{N}{2} \quad (21)$$

with α an arbitrary constant and N the length of the chain. Note that, except for the case of linearly increasing phases, $\Phi_n = \phi n$ ($\phi = \text{constant}$) for which S_n^z will stay constant at all times (this follows directly from Eqs. (7,18)), the inhomogeneity of the phase at $t = 0$ will in general induce a spatial dependence of S_z in the course of time. In the following we choose the phase of the classical and quantum initial state so as to generate two types of excitations: localized states and expanding shock wave solutions.

A) Localized states.

We have generated these excitations with the following initial conditions

- a) $\Phi_n = \phi n$, $n < 0$; $\Phi_n = \phi n + A$, $n \geq 0$; (dislocation),
- b) $\Phi_n = \phi n$, $n \neq 0$; $\Phi_0 = A \neq 0$; (local inhomogeneity).

In Fig. 1 we depict the time evolution of the quantum averaged site magnetization as computed from Eq. (18) for the state in Eq. (11) with phase given by a). In Fig.2 a direct numerical integration of Eq. (7) with a fourth order Runge-Kutta method for the corresponding initial condition in Eq. (20) and Φ_n given by a), is reported. We see that in both cases localized soliton-like excitations are formed together with a radiative field which is much stronger in the case of the classical evolution. The initial conditions of type b) also lead to the formation of soliton-like solutions and background radiation, but in this case the quantum solitons have much shorter life-times and therefore, will not be discussed here.

B) Expanding shock-wave solution.

To form a shock-wave in the magnetization profile we have considered initial conditions of the form $\Phi_n = \phi|n|$, on an infinite open chain (note that the phase has a cusp at $n = 0$). Such a configuration can in principle be prepared by applying a periodic magnetic field $\cos(\omega t)$ to the left half of the chain and a corresponding π -shifted field (i.e. $-\cos(\omega t)$) to the right half. In Figs. 3, 4 we depict the time evolution of this initial condition for, respectively, the quantum and the classical cases. The formation of an expanding symmetrical shock front is clearly seen in both cases and the corresponding time propagations are in a good agreement for long times. We also remark that the expanding inhomogeneous region with higher S_n^z is caused by the fact that there are two opposite fluxes of magnetization $j > 0$ (on the left) and $j < 0$ (on the right), colliding at the center. At the initial time $t = 0$, they are separated by the single site $n = 0$. As time grows, the opposite magnetization currents become separated by the zero-flux region $j \approx 0$, expanding alongside with perturbed S_n^z region as one can see from Fig.5. The symmetry of the S_n^z is just due to the symmetry of the incoming currents.

The relation between the rate of change of magnetization in time and its current is given by a discrete continuity equation

$$\frac{\partial S_n^z}{\partial t} = \langle j_n \rangle - \langle j_{n+1} \rangle, \quad j_n = i \left(s_{n-1}^+ s_n^- - s_{n-1}^- s_n^+ \right), \quad (22)$$

which is obtained from Eq. (2) by averaging with respect to the initial state. Denoting by $-A(t), A(t)$ the boundaries of the perturbed region, and summing Eq. (22) over the points inside this region, we obtain

$$\frac{\partial \sum_{-A(t)}^{A(t)} S_n^z}{\partial t} = \sum_{-A(t)}^{A(t)} (\langle j_n \rangle - \langle j_{n+1} \rangle) = \langle j_{-A(t)} \rangle - \langle j_{A(t)} \rangle. \quad (23)$$

For the case $\Phi_n = \phi|n|$ we find

$$\frac{\partial}{\partial t} \sum_{-A(t)}^{A(t)} S_n^z = \left(1 - (S^z(0))^2 \right) \sin(\phi), \quad (24)$$

from which we see that the excess magnetization in the perturbed S_n^z region grows linearly in time

$$\sum_{-A(t)}^{A(t)} (S_n^z(t) - S_n^z(0)) = \alpha t, \quad \alpha = (1 - (S^z(0))^2) \sin(\phi). \quad (25)$$

Using a similar argument for the local energy

$$E_n = \langle s_n^x s_{n+1}^x + s_n^y s_{n+1}^y \rangle, \quad (26)$$

we obtain that the excess energy inside the perturbed region also increases linearly in time

$$\sum_{-A(t)}^{A(t)} (E_n(t) - E_n^z(0)) = \beta t, \quad \beta = -\frac{1}{4} \left(1 - (S^z(0))^2 \right) S^z(0) \sin(2\phi). \quad (27)$$

This is also seen from Fig.6 where the energy profiles of a shock solution at different instants of time are reported. It is worth to note that the magnetization production is maximal (see Eq. (25) with $\phi = \pi/2$), when the energy production is zero (see Eq. (27)). So, quite surprisingly, the maximal magnetization current is always accompanied by a zero energy current. We observed this feature also in quantum evolution of the XXZ spin hamiltonian, for which the time-dependent Schrödinger problem can be exactly solved for special initial conditions [9]. Another interesting feature of the above solution is its scaling property

$$S_n^z(t) \rightarrow S^z(n/t), \quad n, t \gg 1 \quad (28)$$

for the site magnetization and energy, as well as for the flux and the energy $j_n(t), E_n(t)$, which can be proved along the similar lines as in [8]. Precise form of the scaling function is complicated and is omitted here. Finally, we note that Eq. (28) agrees with Eqs. (25), (27), and that the above scaling properties are shared (numerically, at least) by the classical solution.

V. SUMMARY

In this paper we have compared the exact time evolution of the quantum Heisenberg XY spin 1/2 model with its classical counterpart. In particular, we have reported on localized states and on expanding shock-wave solutions whose classical and quantum evolutions agree for long times. The problem of finding suitable conditions which allow to discriminate the quantum states which will evolve ‘quasiclassically’ from the ones which will not, remains however unsolved. Thus, for example, we found that initial conditions leading to decrease

of absolute value of local magnetization (e.g. initial conditions of Fig. 4 with the sign of ϕ inverted), develop fast instabilities in the classical case which are not observed in the quantum evolution. This could possibly be explained by a difference of the ‘dynamical temperature’ for the classical spin system in the two cases [10]. It will be interesting to extend this analysis to other initial conditions such as the one used in Ref. [11], as well as to other quantum systems such as the XXZ model.

VI. ACKNOWLEDGMENTS

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VII. FIGURE CAPTIONS

Fig.1. Snapshots of site spin-z component s_n^z expectation values for localized excitation at a different moments of time, plotted from Eq. (18). The initial conditions are: $S_z(0) = 0.8$, $\Phi_n = \phi n, n < 0$, $\Phi_n = \phi n + 2\phi, n \geq 0$; $\phi = \pi/2$. Graphs a, b, c, d correspond to time=10, 30, 50, 100 respectively.

Fig.2. the same as in Fig.1 but for the semiclassical evolution obtained from Eq. (7). Graphs b, c, d correspond to time=30, 50, 100 respectively.

Fig.3. Average magnetization profile $\langle s_n^z \rangle$ for shock solution (exact) at different times, computed from Eq. (18). Consecutive expanding curves correspond to $t = 10, 30, 50, 100$. The initial conditions are: $S_z(0) = 0.8$, $\Phi_n = \phi|n|$, $\phi = \pi/4$.

Fig.4. the same as in Fig.3 but for the semiclassical evolution.

Fig.5. Flux profile (exact) at time $t = 0, 30, 50, 100$. Initial conditions are the same as in Fig.3.

Fig.6. Energy profile for a shock solution ($t = 0, 30, 50, 100$). Initial conditions are the same as in Fig.3.

FIGURES

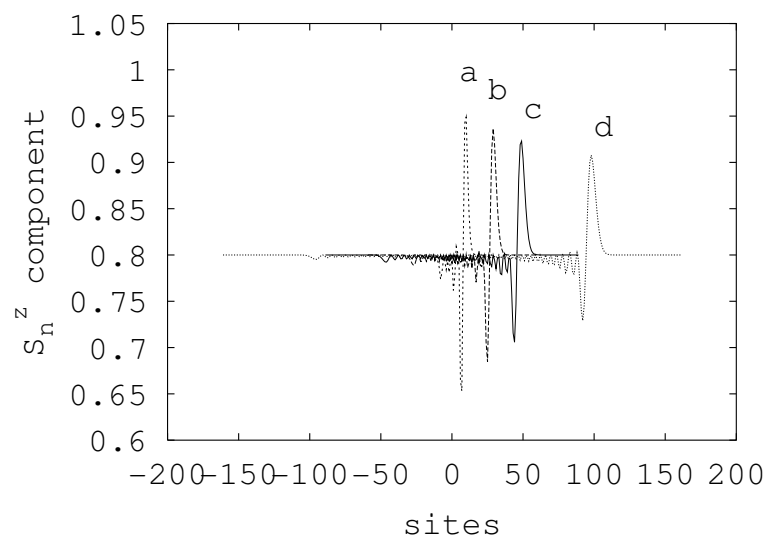


FIG. 1.

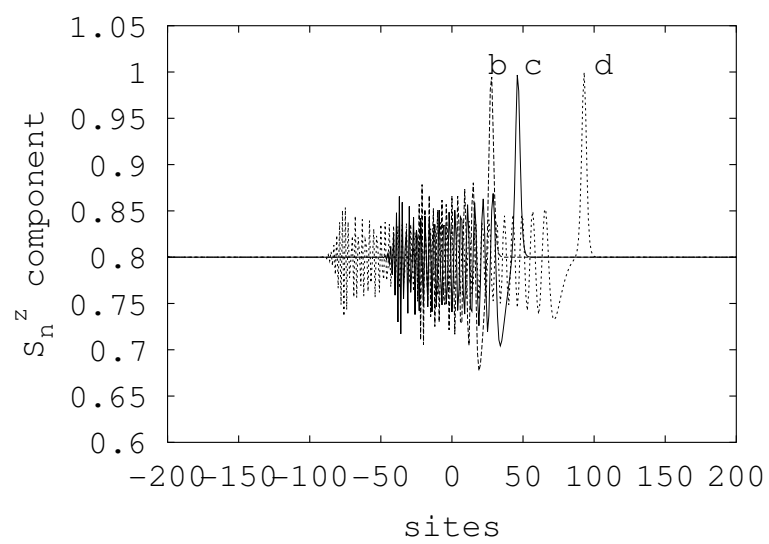


FIG. 2.

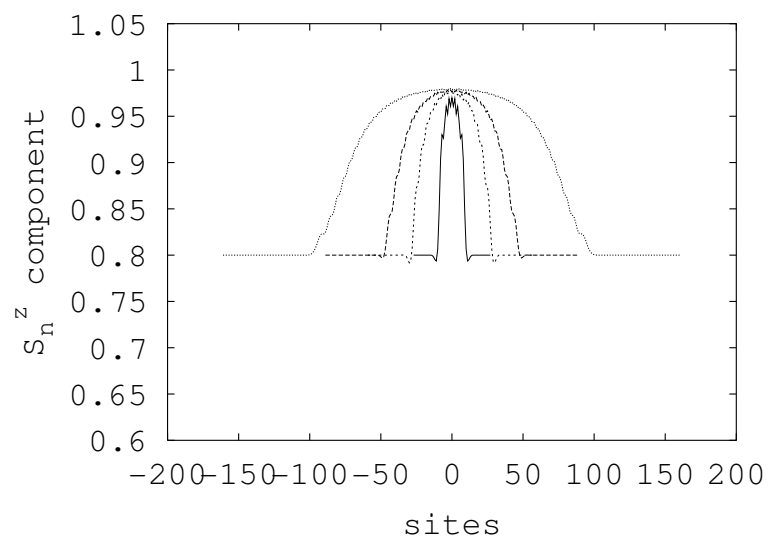


FIG. 3.

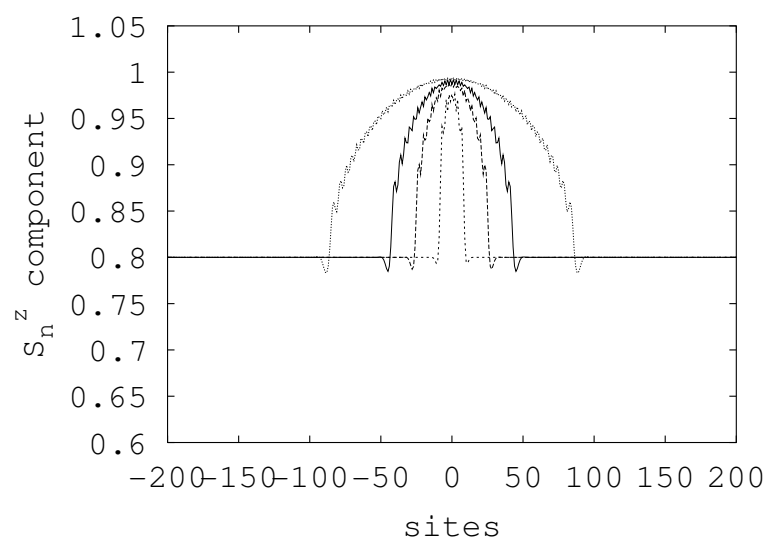


FIG. 4.

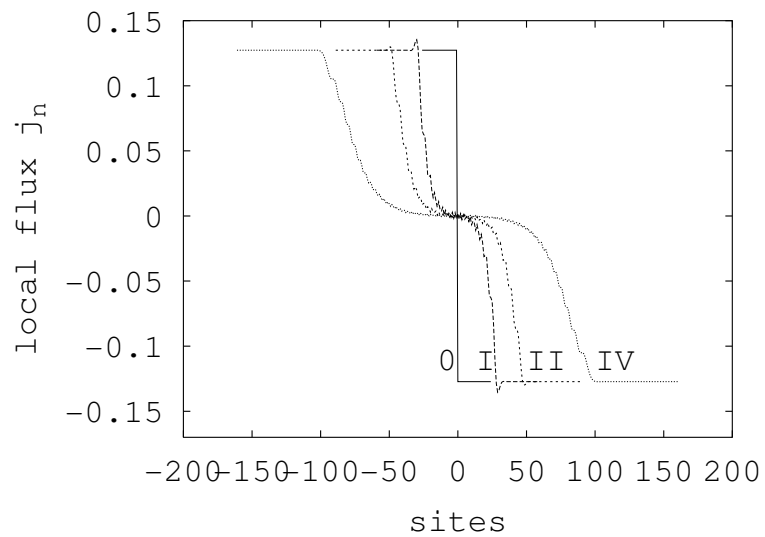


FIG. 5.

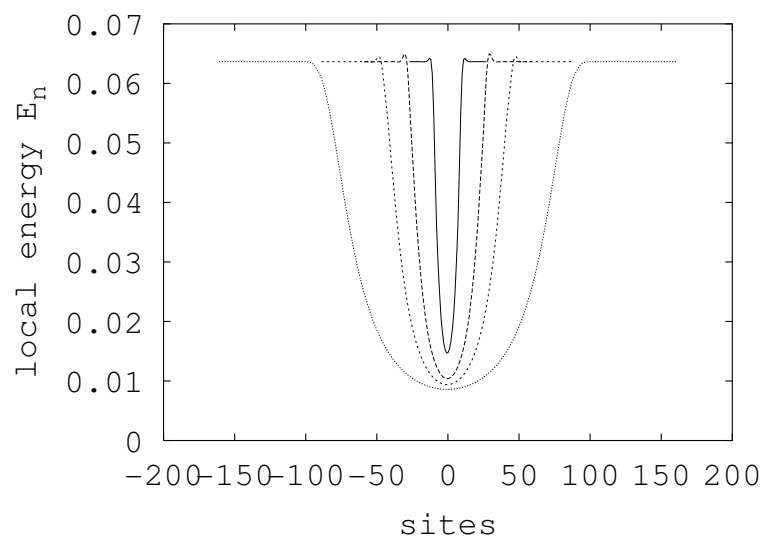


FIG. 6.